

4,4'-Thiodianiline
139-65-1 | DTXSID9021344

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 1.17e-03 mol/L

Global applicability domain: Inside

Local applicability domain index: 4.13e-01

Confidence level: 4.57e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Guanidine, (2-benzothiazolyl)-</div> <div>Measured: 3.62e-03</div> <div>Predicted: 2.64e-03</div>	<div>Image not found</div> <div>Methabenzthiazuron</div> <div>Measured: 2.67e-04</div> <div>Predicted: 1.49e-03</div>	<div>Image not found</div> <div>S-[2-Oxo-2-(phenylamino)ethyl] thiocarbamate</div> <div>Measured: 4.76e-02</div> <div>Predicted: 6.62e-02</div>
<div>Image not found</div> <div>Bis(ethylxanthogen)</div> <div>Measured: 1.14e-05</div> <div>Predicted: 4.06e-05</div>	<div>Image not found</div> <div>Tirpate</div> <div>Measured: 4.27e-03</div> <div>Predicted: 7.86e-03</div>	